ETH
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Computational Quantum Physics
Exercise 12

FS 11
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Problem 12.1 ED impurity solver

In this exercise you will write an impurity solver for the Anderson model with a single bath site that could be used in a DMFT code for the Hubbard model.

1. Write a function which takes the parameters of the AIM $\{U, \mu, \epsilon, V^\sigma\}$ as input and calculates its eigenstates and energies.

2. Write a second function which, given the results of the diagonalization, calculates the imaginary frequency and time Green's functions $G(i\omega_n)$, $G(\tau)$ as well as the self-energy $\Sigma(i\omega_n)$.

The Green's function can be conveniently calculated in the Lehmann representation from the model's eigenstates $|i\rangle$, $|j\rangle$ with eigenenergies E_i, E_j, e.g. in imaginary frequency

$$G_\sigma(i\omega_n) = \frac{1}{Z}\sum_{i,j}\frac{|\langle i|d^\dagger|j\rangle|^2}{i\omega_n + E_i - E_j}\left[\exp(-\beta E_i) + \exp(-\beta E_j)\right], \tag{1}$$

with partition function $Z = \sum_i \exp(-\beta E_i)$ and Matsubara frequencies $\omega_n = (2n+1)\pi/\beta$. The self-energy Σ is extracted from the full Green's function G by comparing to the non-interacting bath Green's function G_0:

$$\Sigma_\sigma(i\omega_n) = G^{-1}_{0,\sigma}(i\omega_n) - G^{-1}_\sigma(i\omega_n), \tag{2}$$

$$G_{0,\sigma}(i\omega_n) = [i\omega_n + \mu - \Delta_\sigma(i\omega_n)]^{-1}, \tag{3}$$

$$\Delta_\sigma(i\omega_n) = \frac{|V|^2}{i\omega_n - \epsilon}. \tag{4}$$

In a DMFT code you would now go on to determine new bath parameters ϵ_p, V_p^σ such that the (local) lattice Green's function matches the impurity Green's function and iterate until self-consistency is reached. (Of course one needs more than one bath sites for a sensible fit).